

4-Pyridinecarboxylic acid, 2-amino-6-chloro-, ethyl ester

Other names:	Ethyl 2-amino-6-chloropyridine-4-carboxylate
Inchi:	InChI=1S/C8H9ClN2O2/c1-2-13-8(12)5-3-6(9)11-7(10)4-5/h3-4H,2H2,1H3,(H2,10,11)
InchiKey:	ZFTAEEJVVVQTXKD-UHFFFAOYSA-N
Formula:	C8H9ClN2O2
SMILES:	CCOC(=O)c1cc(N)nc(Cl)c1
Mol. weight [g/mol]:	200.62
CAS:	28056-05-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.494		Crippen Method
mcvol	139.460	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28056055&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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